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A Dynamic Sampling Approach for Cost Reduction in Semiconductor Manufacturing

Gian Antonio Susto^{a,*}, Marco Maggipinto^a, Federico Zocco^b, Sean McLoone^b

^aUniversity of Padova, Department of Information Engineering, Italy.

^bQueen's University Belfast, Centre For Intelligent Autonomous Manufacturing Systems, United Kingdom.

Abstract

In semiconductor manufacturing, metrology is generally a high cost, non-value added operation that impacts significantly on cycle time. As such, reducing wafer metrology continues to be a major target in semiconductor manufacturing efficiency initiatives. Data-driven spatial dynamic sampling methodologies are here compared. Such strategies aim at minimizing the number of sites that need to be measured across a wafer surface while maintaining an acceptable level of wafer profile reconstruction accuracy. The Spatial Dynamic Sampling approaches are based on analyzing historical metrology data to determine, from a set of candidate wafer sites, the minimum set of sites that need to be monitored in order to reconstruct the full wafer profile using statistical regression techniques. Spatial Dynamic sampling is then implemented in various strategies that guarantee coverage of all the possible sites in a given set of process iteration. In this way, the risk of not detecting previously unseen process behavior is mitigated. In this work, we demonstrate the efficacy of spatial dynamic sampling methodologies using both simulation studies and metrology data from a semiconductor manufacturing process.

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1. Introduction

Measuring important process variables is a critical step in modern days manufacturing, [11], particularly in the semiconductor industry [13], where the manufacturers are in a continuous effort to optimize metrology operations as the complexity of the process rises due to a massive reduction in feature sizes and increase in wafer diameters up to 450 mm. The features of interest, acquired during production, vary depending on the manufacturing process employed, for example, in Chemical Vapor Deposition (CVD) the depth of the material film deposited on the wafer

* Corresponding author.

E-mail address: gianantonio.susto@dei.unipd.it

surface provides important quality information, on the other hand, in plasma etching, the size of the etched trench is an important quality indicator. The spatio-temporal evolution of such features needs to be thoroughly controlled in order to meet the specifications of modern semiconductor devices that become more and more complex as the technology advances. This is usually achieved by means of Advanced Process Control (APC) methodologies that rely on metrology for feedback and/or forward control signals [10]. In the first case, the signals are employed to adjusted the current process operation for the next wafer, in the second case the signals are employed by the next process step in order to compensate for deviations observed in the actual process. In order to provide the necessary information to modern industrial technologies such as the aforementioned APC, but also Predictive Maintenance (PdM) and product quality assessment [12], spatially dense measures would be ideal. However, due to the high costs of metrology operations both in terms of time and money, such high-density measurements are not feasible in practice, since an increase in productions costs would considerably impact the competitiveness on the market. It is thus common practice to reduce the number of required metrology operations both temporally [4] and spatially, [12, 5], to reach a satisfactory trade-off between production quality and costs. Reducing the number of measured locations poses the problem of determining a set of informative sites where the most relevant information on the features of interest resides. Usually, an initial design of the measurement locations is performed either by process engineers, leveraging prior knowledge of the spatial variability over the wafer surface of the signal of interest, or leveraging space filling sampling design techniques such as Latin Hypercube Sampling [16]. Often, during the production process lifetime, previously unseen peculiarities arises and new measurement sites are added to the original set. Such incremental adjustment of the metrology plan often introduces redundancy in the available measurements that can further increase as process issues are solved and the production process is refined. The redundant information introduced in the acquired measurements limits the efficiency of the metrology plan. For this reason, in recent years there has been a boost in adoption of data driven technologies for wafer metrology plan optimization where historical process measurements are leveraged to select a representative sub-set of locations that guarantee a good reconstruction of the feature values at the unmeasured locations exploiting estimation algorithms. In this work we considered the methodology presented in [6] for metrology plan optimization based on Forward Selection Component Analysis (FSCA) [7]. FSCA is a greedy unsupervised selection method that allows a sequential selection of the measurement sites that, leveraging the redundancy in the measurements, provide a good reconstruction of the desired values at the unselected locations through linear regression algorithms. Reducing the sampling plan to a meaningful subset of locations provides an effective way to optimize the metrology costs but there is the risk of missing previously unseen abnormal process evolutions. For this reason, in [5] a set of FSCA-based methods for achieving spatial dynamic sampling have been proposed that guarantee a complete span of the original measurement locations in a limited amount of time while providing good reconstruction performance. In this work, we provide extended simulations and insights into the methodologies presented in [5]. The rest of the paper is organized as follows. A literature review on Dynamic Sampling is provided in Section 2, while the FSCA methodology is described in Section 3. The dynamic sampling extension of FSCA is then explained in Section 4. In Section 5, a description of the industrial dataset and two simulated datasets on which the performance of the proposed method have been estimated are presented. In Section 6 the obtained results are provided, while Conclusions are finally drawn in Section 7.

2. Dynamic Sampling Literature Review

Dynamic sampling methodologies are usually distinguished into two categories: temporal dynamic sampling and spatial dynamic sampling. In the first case, at each process run the system determines whether to measure the wafer at hand or estimate the features of interest by means of an estimation algorithm. In the second case, at each process run the system has to decide which locations on the wafer surface have to be measured and which can be estimated. For the first category, in [3] a method for reducing the number of wafers measured has been proposed, where an ensemble of Artificial Neural Networks (ANNs) has been employed in order to predict the measurement at the wafer being processed based on past measures. Then, if the confidence of the estimated measure (computed over the ensemble of networks) is below a certain threshold the estimation is accepted, otherwise the wafer is physically measured. In [9] a similar approach has been proposed, where a Random Forest (RF) has been employed as the prediction method. The RF is composed of an ensemble of regression/classification tree hence the confidence level can be estimated through the variance of the prediction among them. Moreover, the author proposed a method based on Monte Carlo Cross

Validation (MCCV) in order to obtain a predefined rate of measured wafers. For the second category, Vincent et al. [9] proposed a sampling approach based on Principal Component Analysis and minimum-variance estimation. While the method was designed for both spatial and temporal sampling, the proposed use case was a litho-etch process with spatial evolution. Borgoni et al. [1] proposed a simulated annealing and spatial prediction strategy to optimize the selection of a reduced set of sites from a larger candidate grid for a silicon oxide deposition process. In [14], Zheng addresses the issue of optimal site selection for monitoring and wafer map interpolation of electrical metrology data in the context of developing effective Fault Detection and Classification (FDC) schemes. Four approaches are investigated. Two are supervised selection techniques where sites are sequentially selected based on their utility as inputs for specified wafer classification tasks, and two are unsupervised [8] techniques where the objective is to identify a subset of sites that best represent the remaining sites. The first of the unsupervised approaches is a two-stage methodology where candidate sites are initially clustered using k-means clustering and then a PCA based within-cluster site selection technique employed to select a subset of sites from within each cluster. The second approach involves estimating a bootstrapped forward selection Partial Least Square (PLS) model with measured sites as input and unmeasured sites as outputs to be predicted. Zheng concludes that the two-stage clustering/PCA methodology yields the best FDC performance. In [2], a Gaussian process model based sequential measurement strategy is developed where, for each wafer, an initial set of sites is measured and used to estimate a Gaussian Process (GP) model, which then guides the selection of additional measurements sites to update the GP model until its prediction error on test sites is within an acceptable level. The distinguishing characteristic of this approach is that it does not require historical data for model building, however the number and location of measurement sites change from wafer to wafer, and the need for an initial set of measurements for in-line model estimation means that it is not suited to low measurement density scenarios.

3. FSCA Methodology

Data-driven metrology plan optimization techniques rely on the availability of historical measurements of the features of interest at all the available sites. The data are organized in a so-called design matrix $X \in R^{(N \times V)}$ with $N > V$ where N is the number of available observations (wafers measured) and V is the number of candidate locations on the wafer surface. From now on, x_{ji} will denote the measurement taken at site i on the j^{th} wafer and $x_i \in R^{(N \times 1)}$ will denote the vector of measurements taken at site i for all the available wafers in the dataset. The plan optimization problem is to select the minimum set of sites from the candidate set $I = 1, 2, \dots, V$ that contains most of the information available from the entire set of locations. This can be formulated as selecting a subset of the columns of X that explains most of the variance available in X . This is a well-known problem in Machine Learning (ML) under the name of feature selection. A typical methodology that is employed to quantify the redundancy present in the data is Principal Component Analysis (PCA), a well-known algorithm in the ML community that identifies the directions of maximum variance in the space generated by the rows of the matrix X . If redundancy is present in the data, it is possible to reduce the dimension of the dataset by projecting the rows of X onto the first K directions identified by PCA while keeping most of the available variance. However, each Principal Component is a linear combination of all the column of X it is thus impossible to identify a meaningful subset of columns (measurement locations) that best represent the data.

3.1. FSCA wafer site selection

Selecting the locations that best represent the process variability can be expressed as a combinatorial optimization problem that is known to be NP-Hard. FSCA provides a greedy solution that involves sequentially adding to the measurement set the feature that best represent all the others in polynomial time. In particular, at each step the feature that provides the smallest reconstruction error of the measurement at the unselected locations through linear regression is selected. Specifically, given a column x_i of the matrix X the reconstructed dataset $\hat{X}(x_i)$ can be expressed as:

$$\hat{X}(x_i) = \frac{x_i x_i^T}{x_i^T x_i} X \quad (1)$$

The reconstruction error can be quantified in terms of the Frobenius norm of the difference between the real and reconstructed dataset $\|X - \hat{X}\| = \sum_{(i,j)} (x_{ij} - \hat{x}_{ij})^2$. The resulting algorithm can be formalized as follows, here we assume the columns of X with zero mean: **Input:** X, K , where K is the number of locations to be selected - **Output:** I_{FSC}

1. Initialization: Set $I_{FSC} = \emptyset$, $X_1 = X$ and iteration count $k = 1$.
2. Search: Identify the feature i^* that satisfies $i^* = \underset{i}{\operatorname{argmin}} \|X_k - X_k(x_i)\|_F^2$ and add it to the set of selected sites:
 $I_{FSC} = I_{FSC} \cup i^*$.
3. Deflation: Remove the contribution of x_{i^*} from the matrix X_k : $X_{(k+1)} = X_k - \hat{X}(x_{i^*})$, $k = k + 1$.
4. Repeat: Repeat until $k = K$

4. Dynamic Sampling

The algorithm described in Section 3 provides an effective approach to determining the set of locations that guarantees good performance in terms of profile reconstruction at the unmeasured sites. This approach though, assumes that the whole range of process behaviors is captured in the training data employed, limiting the resilience of the measurement process to the emergence of previously unseen process behavior. To overcome this problem, dynamic sampling procedures can be employed that changes the measurement locations for each processed wafer, thus guaranteeing to periodically visit all the candidate locations. Depending on the algorithm, the periodicity may vary and, moreover, the same algorithm can select more often one site instead of another. To quantitatively characterize this behavior, considering the '*site sampling interval*' as the number of wafer processed without a given site being measured, we define the metric called *Maximum Site Sampling Interval* (MSSI) of a specific algorithm as the largest value among the candidate sites of the site sampling interval. The MSSI can assume a range of values from 0, when a site is measured at every process run to ∞ if a site is never measured. When a new process behavior arises, it is detected with probability 1 if it lasts for more than the MSSI, otherwise it may go undetected. Moreover, as the maximum number of faulty wafers that are processed before a new behavior is detected is equal to the MSSI, it is desirable to keep it as low as possible. Of course, the static metrology plan offered by FSCA presents $MSSI = \infty$ since always the same set of locations is measured. In this paper we provide two cluster based dynamic extensions of FSCA that guarantee $MSSI < \infty$. Of course, employing a location set that differs from the optimal one, negatively impacts the reconstruction performance, a good dynamic algorithm thus provides a satisfactory trade-off between reconstruction performance and MSSI. The rationale behind our method is to assign the V_u unmeasured locations to a cluster generated by the V_m selected sites based on a similarity metric, then, at each process run a location from each cluster C_k $k = 1, \dots, V_m$ is selected sequentially and included in the metrology process. Specifically, the k^{th} location index at time t is determined as:

$$i_k(t) = t \bmod (\operatorname{card}(C_k)) + 1 \quad (2)$$

Various measures of similarity can be employed, in particular here we propose two different approaches: *correlation* and *Normalized Mean Squared Error* (NMSE). The first approach, called Sequential Dynamic Sampling-Correlation (SDS-Corr) is the simplest one and consists of assigning each unmeasured location to the cluster generated by the measured site that it is most correlated with. The second method Sequential Dynamic Sampling-NMSE (SDS-NMSE) consists of assigning each site to the cluster where it produces the smallest increase in prediction error if used instead of the FSCA selected site. This alternative has a much higher computational cost than SDS-Corr. In order to define the impact on prediction performance caused by the substitution, we recall that the reconstruction of the dataset from the columns of the matrix selected by FSCA through linear regression can be expressed as:

$$\hat{X}_u = X_{FSC} (X_{FSC}^T X_{FSC})^{-1} X_{FSC}^T X_u = \phi(X_{FSC}) X_u \quad (3)$$

while the reconstruction of the entire dataset can be expressed as $\hat{X} = \phi(X_{FSC})X$. Then we can define the NMSE as:

$$\mathcal{N}(X_{FSC}) = \frac{\|X - \phi(X_{FSC})X\|_F^2}{\|X - \bar{X}\|_F^2} \times 100 \quad (4)$$

where \bar{X} is the matrix whose column entries are the mean of the corresponding column of the matrix X . The dynamic sampling approach requires different estimation models to be trained for each of the of the unmeasured sites at each process run, this operation can be performed offline and does not impact on the computational complexity of the algorithm. In particular, linear regression will be employed as an estimation algorithm, as preliminary results showed that the introduction of a regularization term does not provide any significant improvement.

5. Case Studies

The proposed dynamic sampling approaches have been tested in three different scenarios: a real dataset provided by an industrial partner and two simulated datasets where the wafer profiles have been artificially generated by means of different of mathematical models.

Industrial Dataset: This consists of the measurements acquired during several weeks of production. The data are related to a production process used in read-write head formation within disk drive semiconductor manufacturing. $N = 316$ wafers have been measured at $V = 50$ available locations.

Simulated Dataset 1: Here the data have been created artificially employing a linear combination of randomly generated Gaussian Radial Basis Functions (RBF) defined on the unit radius disc centered on the origin. In mathematical terms, the surface of each generated wafer can be modeled as follows:

$$z(x, y) = \sum_{i=1}^{N_g} h_i \exp\left(\frac{(x - c_{x_i})^2 + (y - c_{y_i})^2}{S_f^2}\right) + \epsilon \quad (5)$$

where $h_i \sim N(0, 1)$, $c_{x_i}, c_{y_i} \sim U(-1, 1)$, $z(x, y)$ is the profile height at the coordinates (x, y) , and $\epsilon \sim N(0, 0.02)$ is the measurement noise. The number of RBF N_g and the spreading factor S_f can be used to tune the regularity of the functions, in particular the spreading factor adjusts the spatial correlation among the measurements at different locations.

Simulated Dataset 2: In this scenario, the wafer profiles have been generated using a random linear combination of Zernike polynomials, a set of polynomial functions defined on a unit disk that have been widely employed to simulate process with a spatial evolution on circular surfaces. We can define a finite set of Zernike polynomial by means of the degree N and a function Z_n^m parametrized by two indexes n and m , with $n = 0, 1, \dots, N$ and $m = -n, -n+1, \dots, n-1, n$. For a given N the generic Zernike polynomial is indicated with $Z_n^m(\rho, \theta)$ where $\theta \in [0, 2\pi]$, $\rho \in [0, 1]$. For the case study $N = 7$ giving a basis set of 36 Zernike polynomials, denoted as Z_i , $i = 1, 2, \dots, 36$. Wafer surfaces are then generated as: $z(\rho, \theta) = \sum \alpha_i Z_i(\rho, \theta)$ where $\alpha_i \sim N(0, 8 \exp(-0.3i))$.

6. Experimental results

In this section we report the results obtained on the use cases described in Section 5. To obtain a comprehensive statistical description of the models performance we employed Monte Carlo Cross Validation (MCCV), a widely employed technique where the dataset is divided into a training and test dataset, with $N_{test} = qN$ and $N_{train} = N - N_{test}$ where $q \in (0, 1)$, for our purpose $q = 0.33$. The training part is used to train the predictive model while the test part is used to assess its performance. This process is repeated K times and then statistical metrics of the desired performance indicators are computed. Dynamic methods present an inherent trade-off between reconstruction performance and

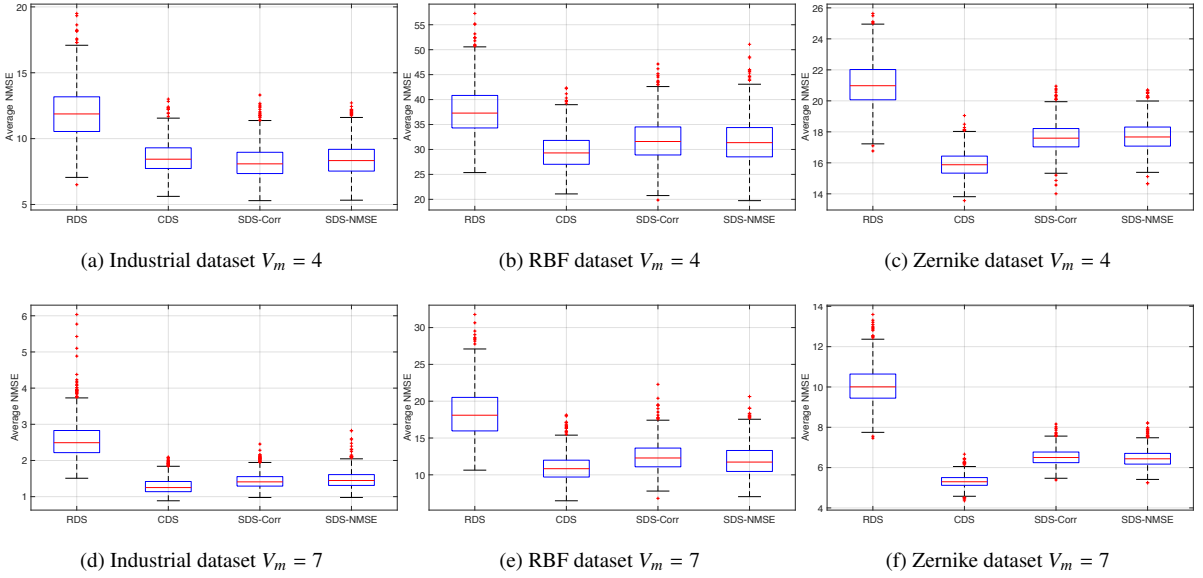


Fig. 1: Boxplot of the NMSE distribution over 1000 MCCV cycles.

duration of the visiting cycle, it is thus important to quantitatively evaluate both these aspects to obtain a complete overview of the performance of the models. Regarding the reconstruction capabilities, the NMSE represents a suitable indicator, while, to quantify the ability of the algorithm to cover the entire wafer with a given number of sites measured V_m , the performance metric Wafer Observability Index (WOI) is introduced. This is defined as:

$$\text{WOI}(V_m) = \frac{\lceil V/V_m \rceil - 1}{\text{MSSI}(V_m)} \times 100 \quad (6)$$

for $V_m < V$. WOI indicates how close $\text{MSSI}(V_m)$ is to the minimum value of the $\text{MSSI} = \lceil V/V_m \rceil - 1$ that can be obtained when the locations are evenly distributed among the V_m clusters.

To provide a performance comparison, we also include in the results two other dynamic methods:

1. Random Dynamic Sampling (RDS): where the sites are ordered randomly and then visited sequentially in blocks of V_m sites.
2. Conservative Dynamic Sampling (CDS): where the first $V_m - 1$ sites are kept constant according to the FSCA selection with the final site is sequentially selected from the unmeasured ones.

In Fig. 1 we report the distribution over $K = 1000$ MCCV cycles of the average NMSE computed with $V_m = 4$ and $V_m = 7$ for the Industrial, RBF and Zernike datasets. The results present an expected behavior, in fact, RDS has the worst performance since it randomly selects the sites without employing any plan optimization algorithm, CDS instead presents the best performance in this case since its deviation from the optimal plan determined by FSCA is minimal; SDS-Corr and SDS-NMSE present similar performances, intermediate with respect to the others.

This behavior is confirmed by Fig. 2 where the curve of the NMSE as a function of the number of selected sites is reported. While such results may suggest that CDS is the best method, this is not true since, as previously stated, an accurate investigation of the number of wafers that need to be processed in order to span the entire wafer surface is required to have a complete overview of the behavior of the algorithms.

Fig 3 shows the median value of the WOI over 1000 MCCV cycles as a function of the number of selected sites. In this case, the RDS has the best performance since it always takes the smallest possible amount of time to visit the

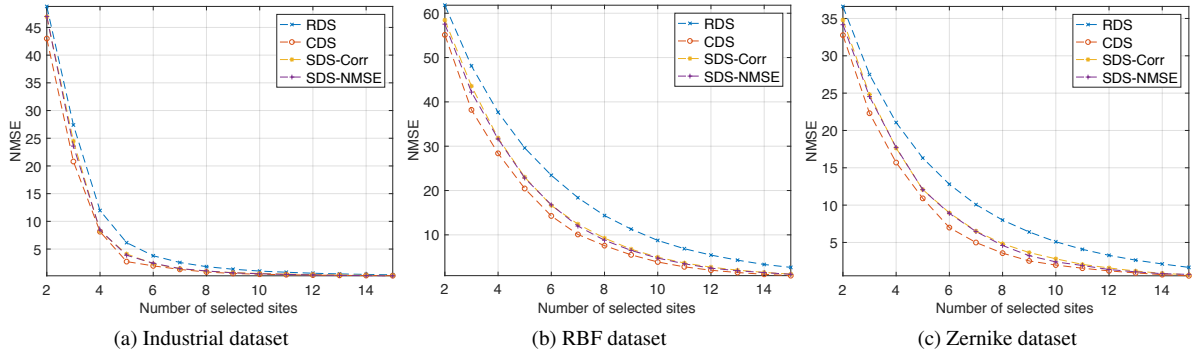


Fig. 2: NMSE as a function of the number of selected sites

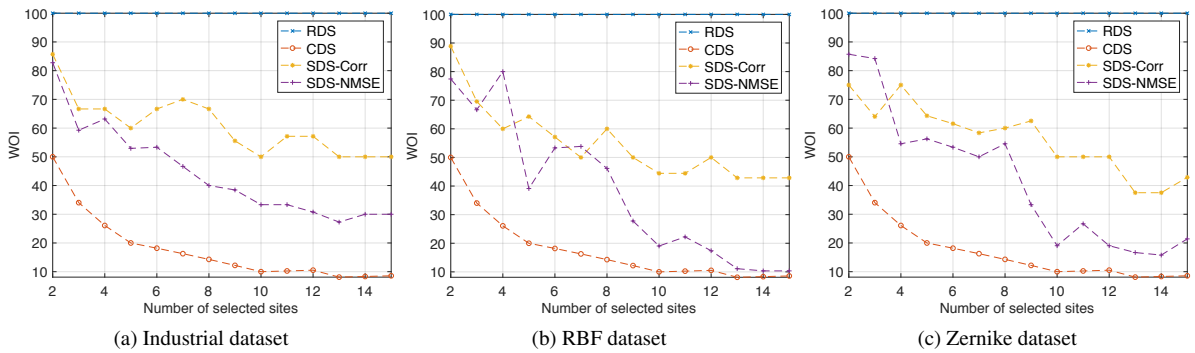


Fig. 3: WOI as a function of the number of selected sites

entire wafer surface. CDS instead presents the worst performance. The SDS methods present similar behavior with $V_m < 6$ while the two curves tend to diverge from each other, with a clear improvement of SDS-Corr w.r.t. SDS-NMSE for $V_m \geq 6$.

We report in Fig 4 the distribution of the number of times that a location is selected per each cycle for the SDS-NMSE and SDS-Corr for $V_m = 4$ and $V_m = 8$. We notice that the SDS-NMSE present high variability on the number of times that a feature is chosen both with $V_m = 4$ and $V_m = 8$ this means that the dimension of the cluster with which the feature is associated, tends to vary more among the validation cycles compared to SDS-Corr.

7. Conclusions

In this paper we presented extended simulation results on dynamic sampling approaches for data-driven metrology plan optimization in the semiconductor manufacturing industries. This problem is of particular importance in such a context where metrology operations are extremely expensive both in terms of time and money. Optimizing the measurement plan has thus a relevant impact on costs management. On the other hand, there is the need to employ dynamic sampling techniques in order to cope with process behaviors that are not captured in the data employed for the data-driven optimization process. The two proposed methods are based on FSCA, a feature selection method that allows the identification, in a greedy fashion, of a subset of significant locations that allow a good reconstruction of the wafer profile at the unmeasured sites through regression techniques. The obtained methodologies, presented a good tradeoff between reconstruction performance and cycle duration, yielding effective metrology plan optimization. In particular, SDS-Corr presents the best choice in terms of WOI; SDS-NMSE provides similar results to SDS-Corr but its cycle duration tends to be higher as the number of selected sites increases.

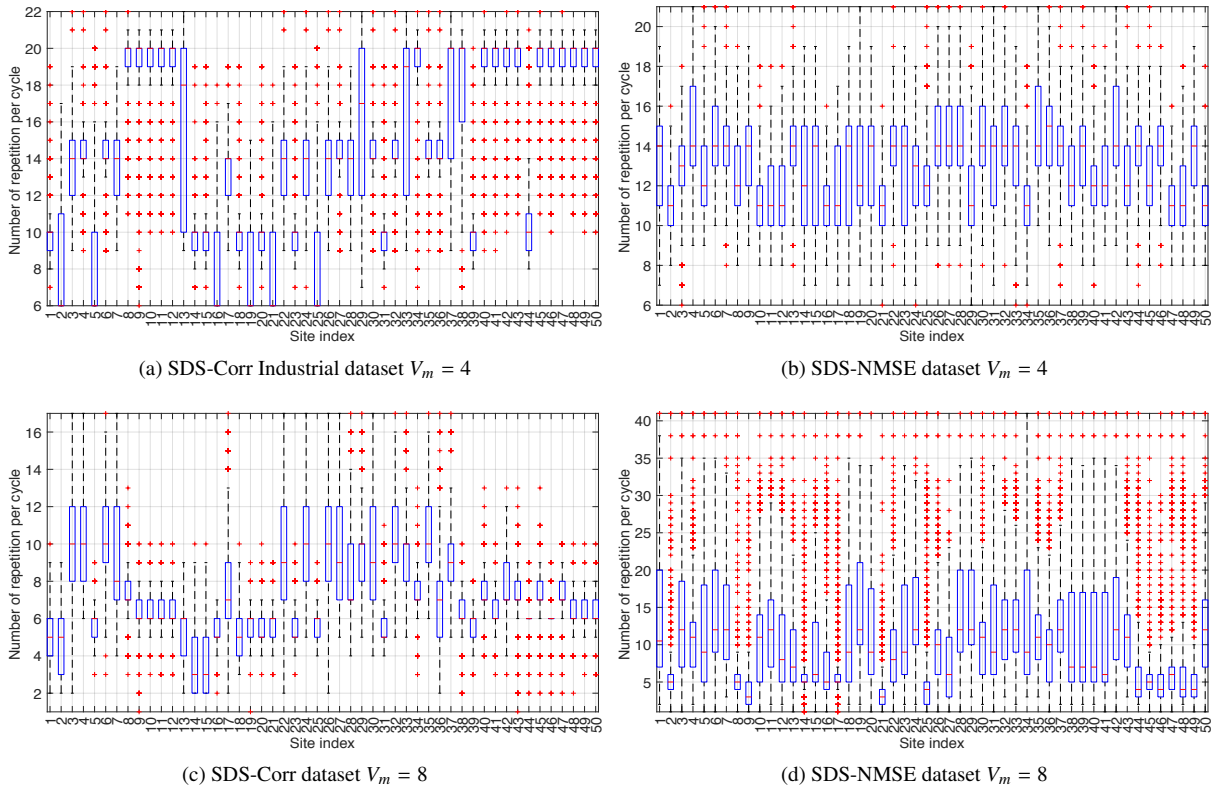


Fig. 4: Distribution of the number of times a site is chosen per cycle for the cluster-based methods.

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